

Volume Elements of Monotone Metrics on the $n \times n$ Density Matrices as Densities-of-States for Thermodynamic Purposes. I

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Among the monotone metrics on the $(n^2 - 1)$ -dimensional convex set of $n \times n$ density matrices, as Petz and Sudár have recently elaborated, there are a *minimal* (Bures) and a *maximal* one. We examine the proposition that it is physically meaningful to treat the volume elements of these metrics as densities-of-states for thermodynamic purposes. In the $n = 2$ (spin- $\frac{1}{2}$) case, use of the maximal monotone metric, in fact, does lead to the adoption of the Langevin (and *not* the Brillouin) function — thus, completely conforming with a recent probabilistic argument of Lavenda. Brody and Hughston also arrived at the Langevin function in an analysis based on the *Fubini-Study* metric. It is a matter of some interest, however, that in the *first* (subsequently modified) version of their paper, they had reported a different result, one fully consistent with the alternative use of the *minimal* monotone metric. In this part I of our investigation, we first study scenarios involving *partially* entangled spin- $\frac{1}{2}$ particles ($n = 4, 6, \dots$), and then a certain three-level extension of the two-level systems. In part II, we examine, in full generality, and with some limited analytical success, the cases $n = 3$ and 4.

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I. INTRODUCTION

The Horodecki's have recently studied [1,2] the relationship between quantum entanglement and the Jaynes inference scheme based on the maximization of entropy [3–5]. They found that the Jaynes methodology “can lead to problems with processing of entanglement”. In this study, we also examine connections between the entanglement of quantum systems and their statistical/thermodynamic properties, but from a rather different viewpoint (cf. [6]). A principal motivation for us in undertaking this work has been the recent contention of Brody and Hughston [7] that the

conventional (Jaynes) density-matrix approach to the canonical ensemble is semiclassical in certain respects (since it eliminates the weighting of the quantum phase space volume), along with their accompanying presentation of an alternative “quantum canonical ensemble” based on the metrical geometry of this space. In particular, Brody and Hughston analyzed the case of a spin- $\frac{1}{2}$ particle in a heat bath and arrived (in the *first* version [8] of their paper [7]) at the partition function,

$$Q(\beta) = 2\sqrt{\pi}\Gamma(\frac{3}{2})(\beta h)^{-1}I_1(\beta h) = \pi(\beta h)^{-1}I_1(\beta h). \quad (1)$$

Here, $\beta = \frac{1}{kT}$ is the inverse temperature (T being temperature), k is Boltzmann’s constant, h is the magnetic field, and $I_1(x)$ is a particular modified (hyperbolic) Bessel function ($I_\nu(x), \nu = 1$) of the first kind. (Such functions often appear in the distribution of spherical and directional random variables [9].) From (1), one can derive the expectation of the energy [8, eq. (14)],

$$E = -\frac{\partial \log Q(\beta)}{\partial \beta} = -\frac{hI_2(\beta h)}{I_1(\beta h)} = -\mu B \frac{I_2(\mu B/kT)}{I_1(\mu B/kT)}, \quad (2)$$

where μ is the particle’s magnetic moment, and B is the external magnetic field strength, with $h \equiv \mu B$. (Ratios of modified Bessel functions, such as appear in (2), play “an important role in Bayesian analysis” [9]. In the limit $\beta \rightarrow 0$, the expected value of the energy (2) is 0, while the variance about the expected value is, then, $\frac{h^2}{4}$.) The *semiclassical* analogue of (2) is the Brillouin function [6],

$$E = -h \frac{I_{\frac{1}{2}}(\beta h)}{I_{-\frac{1}{2}}(\beta h)} = -h \tanh \beta h. \quad (3)$$

Not only have Brody and Hughston expressed certain reservations and qualifications regarding the Brillouin function, so has Lavenda [10, p. 193]. He argued that the “Brillouin function has to coincide with the first moment of the distribution [for a two-level system having probabilities $\frac{e^x}{e^x+e^{-x}}$ and $\frac{e^{-x}}{e^x+e^{-x}}$, where $x = \frac{\mu B}{kT}$], and this means that the generating function is $Z(x) = \cosh x$. Now, it will be appreciated that this function can not be written as a definite integral, such as

$$Z(\beta) = \frac{1}{2} \int_{-1}^1 e^{\beta x} dx = \frac{\sinh \beta}{\beta} = (\frac{\pi}{2\beta})^{\frac{1}{2}} I_{\frac{1}{2}}(\beta), \quad (4)$$

because the integral form for the hyperbolic Bessel function,

$$I_\nu(x) = \frac{(x/2)^\nu}{\sqrt{\pi}\Gamma(\frac{1}{2} + \nu)} \int_{-1}^1 e^{\pm xt} \sin t^{\nu-\frac{1}{2}} dt, \quad (5)$$

exists only for $\nu > \frac{1}{2}$. This means that $I_{-\frac{1}{2}}(x) = (\frac{2}{\pi x})^{\frac{1}{2}}$ cannot be expressed in the above integral form. Since the generating function cannot be derived as the Laplace transform of a prior probability density, it casts serious doubts on the probabilistic foundations of the Brillouin function. In other words, any putative expression for the generating function must be compatible with the underlying probabilistic structure; that is, it must be able to be represented as the Laplace transform of a prior probability density” (see also the further detailed remarks of Lavenda, to much the same effect [10, pp. 20, 198]). Since the model yielding (1) and (2) is based on the integral form for $I_\nu(x)$, for $\nu = 1 > \frac{1}{2}$, it clearly accords with the requirements of Lavenda.

Brody and Hughston [7] raised the possibility that the quantum canonical ensemble could be distinguished from the conventional canonical ensemble by a suitable measurement on a sufficiently *small* quantum mechanical system. In such a case, they argued there would not seem to be any *a priori* reason for adopting the semiclassical mixed state approximation, which allows random phases to be averaged over. Park and Band, in an extended series of papers [11], expressed various qualms regarding the conventional (Jaynes) approach. Park [12] himself later wrote that “the details of quantum thermodynamics are presently unknown” and “perhaps there is more to the concept of thermodynamic equilibrium than can be captured in the canonical density operator itself.” Friedman and Shimony [13], in a classical rather than quantum context, claim to have “exhibited an anomaly in Jaynes’ maximum entropy prescription”.

The (initially presented) results of Brody and Hughston [8], that is, (1) and, implicitly, (2), had, in fact, been reported somewhat earlier by Slater [14], along with parallel formulas for the *quaternionic* two-level systems, in particular, the partition function (cf. (1)),

$$Q(\beta) = 4\sqrt{\pi}\Gamma(\frac{5}{2})(\beta h)^{-2}I_2(\beta h) = 3\pi(\beta h)^{-2}I_2(\beta h)/4. \quad (6)$$

This other analysis [14], similarly to [7], relied upon a metrical geometry, but the two approaches pursued appear, at least superficially, to be somewhat different. The work of Brody and Hughston employed the *Fubini-Study* metric on the complex projective space CP^n (the space of rays — which they regarded as the “true ‘state space’ of quantum mechanics”). The study of Slater, on the other hand, utilized the *Bures* metric, which is defined on the space of density matrices [17–19]. However, Petz and Sudár [15] have recently shown that the extension of the Bures metric to the pure states is exactly the Fubini-Study metric, and that, in point of fact, the Bures metric is the only *monotone* metric which admits such an extension. (The Bures metric is the *minimal* monotone metric [15]. The Bures distance — known also as the Hellinger or Kakutani inner product — is defined as an inner product of two probability measures on some measurable space [20]. Therefore, it can be naturally defined on the space of pure states, namely, CP^n .) So, these two approaches may be demonstrably fully consistent with one another — as their agreement in yielding the results (1) and (2) might lead one to hypothesize. However, we must bear in mind that Brody and Hughston were led, in the second version of their paper [7], to revise certain of their original conclusions [8], in the manner indicated at the beginning of sec. IV. (In their several recent joint papers dealing with quantum statistical issues, Brody and Hughston have chosen to “emphasize the role of the space of *pure* quantum states, since in the Hilbert space based classical-quantum statistical correspondence this is the state space that arises as the immediate object of interest. In fact, the space of density matrices has a very complicated structure, owing essentially to the various levels of ‘degeneracy’ a density matrix can possess, and the relation of these levels to one another” [16].)

In the present communication, we follow in sec. II the specific line of argument of Slater [14] (based on the Bures metric), with the objective of developing “quantum canonical ensembles” for higher-dimensional situations than the (two-dimensional) one presented by a single spin- $\frac{1}{2}$ particle, previously analyzed. We examine several different scenarios for partially entangled spin- $\frac{1}{2}$ particles, and conduct an analysis of the same nature in sec. III for a certain *three*-level extension of the two-level systems, previously studied [21]. Then, in sec. IV, we reexamine the scenarios studied in sec. II, but now with the use of the *maximal* rather than minimal monotone metric. In an appendix, we report information gains from possible outcomes of joint measurements of the partially entangled spin- $\frac{1}{2}$ particles.

We would also like to bring to the reader’s attention, the second part of this study [22], in which certain results (indicated in sec. V, based on the *maximal* monotone metric, the subject of sec. IV) of a surprisingly simple nature have been obtained for the most general (unrestricted) form of scenario for a spin-1 particle (describable by a 3×3 density matrix with eight free parameters). In [22], we also derived some results pertaining to the (yet unrealized) possibility of extending the form of analysis taken there to general spin- $\frac{3}{2}$, or equivalently *arbitrarily* coupled or entangled spin- $\frac{1}{2}$ systems (describable by a 4×4 density matrix with fifteen free parameters). (We are confronted there with a challenging problem of diagonalizing a 6×6 symmetric matrix.)

II. ANALYSES BASED ON THE MINIMAL MONOTONE (BURES) METRIC

In general, the 4×4 density matrix $(\rho^{(a,b)})$ of a pair of (arbitrarily entangled) spin- $\frac{1}{2}$ particles (a, b) can be written in the form (we adopt the notation of [23]),

$$\rho^{(a,b)} = \frac{1}{4}\{I^{(a)} \otimes I^{(b)} + \xi^{(a)}\sigma^{(a)} \otimes I^{(b)} + I^{(a)} \otimes \xi^{(b)}\sigma^{(b)} + \sum_{i,j=1}^3 \zeta_{ij}\sigma_i^{(a)} \otimes \sigma_j^{(b)}\}, \quad (7)$$

where $I^{(a),(b)}$ and $\sigma^{(a),(b)}$ are Pauli matrices acting in the space of particle a and b , respectively. The three-vectors $\xi^{(a),(b)}$, where $\xi^{(a)} = (\xi_1^{(a)}, \xi_2^{(a)}, \xi_3^{(a)})$, correspond (in the case of photons) to the Stokes vectors, while the parameters ζ_{ij} describe the interparticle correlations. If the two particles are independent (nonentangled), then, $\zeta_{ij} = \xi_i^{(a)}\xi_j^{(b)}$. In all the scenarios considered below, it is assumed that particle a is described by the same 2×2 density matrix as particle b , that is, $\rho^{(a)} = \rho^{(b)}$, or equivalently, $\xi^{(a)} = \xi^{(b)}$.

A. Particles a and b are Polarized and Correlated with Respect to the Same Direction

For the first of several scenarios to be examined, let us set twelve of the fifteen parameters in the expansion (7) *ab initio* to zero, leaving only: (1) $\xi_1^{(b)}$, which we equate to $\xi_1^{(a)}$; and (2) ζ_{11} . This corresponds to a situation in which the two particles are unpolarized and uncorrelated except in one direction (associated with the index “1”) of three

underlying orthogonal directions. Thus, we are concerned with a *doubly*-parameterized set of 4×4 density matrices. These have the eigenvalues,

$$\frac{1 - \zeta_{11}}{4}, \quad \frac{1 - \zeta_{11}}{4}, \quad \frac{1}{4}(1 + 2\xi_1^{(a)} + \zeta_{11}), \quad \frac{1}{4}(1 - 2\xi_1^{(a)} + \zeta_{11}) \quad (8)$$

and corresponding eigenvectors,

$$(0, 0, 1, 0), \quad (0, 1, 0, 0), \quad (1, 0, 0, 0), \quad (0, 0, 0, 1) \quad (9)$$

(Such a system is in a state of degeneracy if either $\zeta_{11} = 1$ or $\zeta_{11} = -1 \pm 2\xi_1^{(a)}$, since at least one of the eigenvalues is, then, zero. For the system to be in a pure state, we must have $\zeta_{11} = 1$ and $\xi^{(a)} = \pm 1$.) We employed these results ((8), (9)) in the formula of Hübner [17] for the Bures metric,

$$d_B(\rho, \rho + d\rho)^2 = \sum_{i,j=1}^n \frac{1}{2} \frac{|\langle i | d\rho | j \rangle|^2}{\lambda_i + \lambda_j}, \quad (10)$$

where λ_i is the i -th eigenvalue and $\langle i |$ the corresponding eigenvector of an $n \times n$ density matrix ρ . For the case at hand, we have the result,

$$d_B(\rho, \rho + d\rho)^2 = g_{\xi_1^{(a)} \xi_1^{(a)}} d\xi_1^{(a)2} + g_{\xi_1^{(a)} \zeta_{11}} d\xi_1^{(a)} d\zeta_{11} + g_{\zeta_{11} \zeta_{11}} d\zeta_{11}^2, \quad (11)$$

where

$$g_{\xi_1^{(a)} \xi_1^{(a)}} = \frac{1 + \zeta_{11}}{2(-4\xi_1^{(a)2} + (1 + \zeta_{11})^2)}, \quad (12)$$

$$g_{\xi_1^{(a)} \zeta_{11}} = \frac{\xi_1^{(a)}}{4\xi_1^{(a)2} - (1 + \zeta_{11})^2}, \quad (13)$$

and

$$g_{\zeta_{11} \zeta_{11}} = \frac{1 - 2\xi_1^{(a)2} + \zeta_{11}}{4(-1 + 2\xi_1^{(a)} - \zeta_{11})(-1 + \zeta_{11})(1 + 2\xi_1^{(a)} + \zeta_{11})}. \quad (14)$$

The corresponding volume element of the Bures metric is (cf. [24])

$$\sqrt{g_{\xi_1^{(a)} \xi_1^{(a)}} g_{\zeta_{11} \zeta_{11}} - \left(\frac{g_{\xi_1^{(a)} \zeta_{11}}}{2}\right)^2} = \frac{1}{2\sqrt{2}} \sqrt{\frac{1}{(-1 + 2\xi_1^{(a)} - \zeta_{11})(-1 + \zeta_{11})(1 + 2\xi_1^{(a)} + \zeta_{11})}}. \quad (15)$$

If we integrate this volume element, first, over $\xi_1^{(a)}$ from $-\frac{1}{2} - \frac{\zeta_{11}}{2}$ to $\frac{1}{2} + \frac{\zeta_{11}}{2}$ and, then, over ζ_{11} from -1 to 1, we obtain the result $\frac{\pi}{2}$. (These limits define the domain of feasible values of $\xi_1^{(a)}$ and ζ_{11} — which determine a triangular region — for our doubly-parameterized density matrix. Outside this region, not all the eigenvalues of $\rho^{(a,b)}$ lie between 0 and 1, as they must.) Dividing (15) by $\frac{\pi}{2}$, we obtain a (prior) probability distribution [25] over the domain of these doubly-parameterized 4×4 density matrices. Again, integrating the resultant probability distribution over $\xi^{(a)}$, between the same limits as before, we obtain a univariate probability distribution,

$$i \frac{\log(1 + \zeta_{11}) - \log(-1 - \zeta_{11})}{2\pi\sqrt{2}\sqrt{1 - \zeta_{11}}}, \quad (16)$$

over the interval $\zeta_{11} \in [-1, 1]$. If we now regard (16) as a (normalized) structure function or density-of-states for thermodynamic purposes, multiply it by a Boltzmann factor, $e^{-\beta h \zeta_{11}}$, and integrate over ζ_{11} from -1 to 1, we obtain the partition function,

$$Q(\beta) = \frac{e^{-\beta h} \sqrt{\pi} \operatorname{erfi}(\sqrt{2\beta h})}{2\sqrt{2\beta h}}, \quad (17)$$

where erfi denotes the imaginary error function $\frac{\text{erf}(iz)}{i}$. (The error function $\text{erf}(z)$ is the integral of the Gaussian distribution, that is, $\frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$.) For the expected value of the “energy” ($h\zeta_{11}$), we have, then,

$$-\frac{\partial \log Q(\beta)}{\partial \beta} = \frac{1}{2\beta} + h - \frac{h\sqrt{2}e^{2\beta h}}{\text{erfi}(\sqrt{2\beta h})\sqrt{\pi\beta h}}. \quad (18)$$

As $\beta \rightarrow 0$, this expected value approaches $\frac{h}{3}$, while the variance about the expected value approaches $\frac{16h^2}{45}$.

If we choose in this scenario to first integrate the volume element (15) over ζ_{11} (rather than $\xi_1^{(a)}$) from $-1 - 2\xi_1^{(a)}$ to $-1 + 2\xi_1^{(a)}$, then we obtain (where K represents the complete elliptic integral of the first kind),

$$\frac{K\left(\frac{2\xi_1^{(a)}}{\xi_1^{(a)}+1}\right)}{2\sqrt{-\xi_1^{(a)}-1}}, \quad (19)$$

which can not be explicitly integrated over $\xi_1^{(a)}$ from -1 to 1 (nor if, first, multiplied by a Boltzmann factor, $e^{-\beta h \xi_1^{(a)}}$).

B. Particles a and b are Polarized and Uncorrelated in One Direction, Unpolarized and Correlated in An Orthogonal Direction

Let us modify the previous scenario (sec II A) slightly by now setting the formerly free parameter ζ_{11} to 0, and letting ζ_{22} be free instead. We still maintain $\xi_1^{(b)} = \xi_1^{(a)}$, with the remaining twelve parameters once again set to zero. This corresponds to a situation in which the particles a and b are correlated in one particular direction (labeled “2”), but unpolarized in that direction. The elements of the Bures metric are, then,

$$g_{\xi_1^{(a)} \xi_1^{(a)}} = \frac{-1 + \zeta_{22}^2}{2(-1 + 4\xi_1^{(a)2} + \zeta_{22}^2)}, \quad (20)$$

$$g_{\xi_1^{(a)} \zeta_{22}} = \frac{\xi_1^{(a)} \zeta_{22}}{1 - 4\xi_1^{(a)2} - \zeta_{22}^2}, \quad (21)$$

and

$$g_{\zeta_{22} \zeta_{22}} = \frac{1 - \zeta_{22}^2 + 2\xi_1^{(a)2}(-2 + \zeta_{22}^2)}{4(-1 + \zeta_{22}^2)(-1 + 4\xi_1^{(a)2} + \zeta_{22}^2)}. \quad (22)$$

The integrations of the corresponding volume element of the Bures metric ((20)-(22)) are now performed, first, over $\xi_1^{(a)}$ from $-\frac{\sqrt{1-\zeta_{22}^2}}{2}$ to $\frac{\sqrt{1-\zeta_{22}^2}}{2}$ and, then, over ζ_{22} from -1 to 1. (The feasible values lie within an ellipse, the equation of which is $4\xi_1^{(a)2} + \zeta_{22}^2 = 1$.) This gives us a result of $\frac{\pi}{2\sqrt{2}}$, which we can use to obtain a normalized volume element, that is, a (prior) probability distribution,

$$\frac{1}{\pi\sqrt{1 - 4\xi_1^{(a)2} - \zeta_{22}^2}}, \quad (23)$$

over the domain of the doubly-parameterized 4×4 density matrices for this scenario. The univariate marginal distribution of (23) over $\zeta_{22} \in [-1, 1]$ is simply uniform ($\frac{1}{2}$) — which we take as our (normalized) structure function. Applying the Boltzmann factor, $e^{-\beta h \zeta_{22}}$ to it, gives us a partition function (cf. (4)),

$$Q(\beta) = \frac{\sinh \beta h}{\beta h} = \left(\frac{\pi}{2\beta h}\right)^{\frac{1}{2}} I_{\frac{1}{2}}(\beta h), \quad (24)$$

yielding an expected value of the “energy” ($h\zeta_{22}$) equal to

$$-\frac{\partial \log Q(\beta)}{\partial \beta} = -h \frac{I_{\frac{3}{2}}}{I_{\frac{1}{2}}} = \frac{1}{\beta} - h \coth \beta h. \quad (25)$$

(In the limit $\beta \rightarrow 0$, this expected value approaches 0, while the corresponding variance approaches $\frac{h^2}{3}$.) It should be noted that the results (24) and (25) are formally equivalent to those given by the Langevin model of paramagnetism [26].

C. Particles a and b are Polarized and Uncorrelated in One Direction, Unpolarized and Equally Correlated in the Two Orthogonal Directions

The only difference between this scenario and the previous one (sec. II B) is that the correlation ζ_{33} is not set to 0, but rather equated to ζ_{22} . (So, although the particles a and b are unpolarized in the third direction, the outcomes of their individual spin measurements in this direction may be correlated with one another.) This leads to a more simple outcome. The normalized form of the Bures volume element is, now,

$$\frac{4}{\pi^2 \sqrt{1 - 4\xi_1^{(a)^2}} \sqrt{1 - 4\zeta_{22}^2}}. \quad (26)$$

The domain of feasible values is the square defined by the lines $\xi_1^{(a)} = \pm \frac{1}{2}$ and $\zeta_{22} = \pm \frac{1}{2}$. (So, the bivariate probability distribution (26) factors into the product of two univariate probability distributions.) We can, then, multiply (26) by the bivariate Boltzmann factor $e^{-\beta \xi h \xi_1^{(a)} - \beta \zeta h \zeta_{22}}$ and integrate over the square region to obtain the (product) partition function,

$$Q(\beta_\xi, \beta_\zeta) = I_0\left(\frac{\beta_\xi h}{2}\right) I_0\left(\frac{\beta_\zeta h}{2}\right). \quad (27)$$

We have also obtained partition functions of the form $I_0(\frac{\beta h}{2})$ in two quite different scenarios, in which we set thirteen of the fifteen parameters in the expansion (7) to zero and, otherwise, set the cross-correlation ζ_{21} equal to either ζ_{12} or to $-\zeta_{12}$.

D. Particles a and b are Unpolarized, but Equally Correlated in Three Orthogonal Directions

In this scenario, we set the six components of the two vectors $\xi^{(a)}$ and $\xi^{(b)}$ to zero, so the particles a and b are assumed to be unpolarized in each of the three orthogonal directions (and, thus, with respect to any arbitrary orientation). We also fix $\zeta_{ij} = 0$ if $i \neq j$, so there are no correlations between spin measurements in different directions. (So, in these respects, a and b are independent or nonentangled.) Finally, we set $\zeta_{33} = \zeta_{22} = \zeta_{11}$, so correlations are allowed between the measurements of a and b in the same direction. Thus, we are concerned here, not with a doubly-parameterized family as in the first two analyses, but with a singly-parameterized one.

We obtain as our prior probability distribution over the feasible range $\zeta_{11} \in [-1, 1/3]$,

$$\frac{\sqrt{3}}{\pi \sqrt{1 - 3\zeta_{11}} \sqrt{1 + \zeta_{11}}}, \quad (28)$$

from which one obtains the partition function,

$$Q(\beta) = e^{\frac{\beta h}{3}} I_0\left(\frac{2\beta h}{3}\right), \quad (29)$$

and an expected value of the “energy” ($h\zeta_{11}$) of

$$-\frac{\partial \log Q(\beta)}{\partial \beta} = \frac{h}{3} \left(-1 - \frac{2I_1(\frac{2\beta h}{3})}{I_0(\frac{2\beta h}{3})}\right). \quad (30)$$

So, we again encounter a ratio of modified Bessel functions (cf. (2)) [9]. The value of (30) at $\beta = 0$ is $-\frac{h}{3}$ while that of the associated variance is the square of this, that is $\frac{2h^2}{9}$.

E. Three and More Unpolarized Particles having Equal Highest-Order Intradirectional Correlations

The first of several scenarios discussed in this section might be regarded as a *three*-particle (a, b, c) analogue of the two-particle one presented in the immediately preceding section (IID). For a general 8×8 density matrix ($\rho^{a,b,c}$) representing the joint state of the three particles, we have an expansion analogous to (7). In this expansion, we consider all the 63 parameters to equal 0, except for the three ($\zeta_{111}, \zeta_{222}, \zeta_{333}$) representing the highest-order intradirectional correlations. We regard these three parameters as having a common value, which is designated ζ_{111} . In other words, there is a possibly nonzero correlation between the outcomes of spin measurements in some fixed direction for the three particles.

The normalized volume element of the corresponding Bures metric is, then,

$$\frac{\sqrt{8\zeta_{111}^2 - 3}}{E(\frac{8}{9})\sqrt{12\zeta_{111}^2 - 4}}, \quad (31)$$

where E represents the complete elliptic integral, and the range of feasible values is $\zeta_{111} \in [-1/\sqrt{3}, 1/\sqrt{3}]$. However, no explicit formula for the partition function was found.

Let us continue this line of analysis to the *four*-particle case. Now, there are 255 parameters in the expansion analogous to (7). We set 252 of them to 0, and equate both of the correlations ζ_{2222} and ζ_{3333} to ζ_{1111} , so again we are concerned with a singly-parameterized family of density matrices. The feasible range of ζ_{1111} is the interval $[-1/3, 1]$. We are able to normalize the volume element of the Bures metric over this interval, obtaining the probability distribution (cf. (28)),

$$\frac{\sqrt{3}}{\pi\sqrt{1 - \zeta_{1111}}\sqrt{1 + 3\zeta_{1111}}}, \quad (32)$$

and the partition function (cf. (29))

$$Q(\beta) = e^{-\frac{\beta h}{3}} I_0\left(\frac{2\beta h}{3}\right), \quad (33)$$

giving an expected value of the “energy” ($h\zeta_{1111}$) (cf. (30)),

$$-\frac{\partial \log Q(\beta)}{\partial \beta} = \frac{h}{3} \left(1 - \frac{2I_1(\frac{2\beta h}{3})}{I_0(\frac{2\beta h}{3})}\right). \quad (34)$$

For $\beta = 0$, this expected value equals $\frac{h}{3}$, while the associated variance is $\frac{2h^2}{9}$.

For the *five*-particle analogue, the thermodynamic behavior was precisely the same as for the three-particle case discussed just above (31), with the replacement of ζ_{111} by ζ_{11111} . For the *six*-particle analogue, the same results ((28)-(30)) were obtained as in the *two*-particle case of sec. IID (replacing ζ_{11} by ζ_{111111}).

F. Three Unpolarized Particles having Equal *Second* Highest-Order Intradirectional Correlations

We modify the scenarios of the previous section (IIE) by, now, requiring the highest-order correlations to be 0, while equating all the second-order correlations to each other, obtaining, thereby, the one free parameter. In the three particle case, there are nine such correlations — the assumed common value of which, we denote by ζ_{110} . The corresponding prior probability distribution over the feasible range $\zeta_{110} \in [-1/3, 1/3]$ is, then,

$$\frac{6}{\pi(4 - 36\zeta_{110}^2)}, \quad (35)$$

yielding a partition function,

$$Q(\beta) = I_0\left(\frac{\beta h}{3}\right). \quad (36)$$

The expected value of the “energy” ($h\zeta_{110}$) is,

$$-\frac{\partial \log Q(\beta)}{\partial \beta} = -\frac{h}{3} \frac{I_1(\frac{\beta h}{3})}{I_0(\frac{\beta h}{3})}. \quad (37)$$

For $\beta = 0$, this is equal to 0, with a corresponding variance of $\frac{h^2}{18}$.

In the four-particle analogue, we have twelve second-highest order correlations — the assumed common value of which, denoted ζ_{1110} , has a feasible range of $[-\frac{1}{4\sqrt{3}}, \frac{1}{4\sqrt{3}}]$. However, we have been unable to determine the set of eigenvectors to employ in the formula (10), and, thereby, can not further pursue the analysis. Interestingly though, we have been able to determine the eigenvalues and eigenvectors for the five-particle analogous scenario — in which the single parameter ζ_{11110} must lie in the interval $[-\frac{1}{7}, \frac{1}{5}]$. The volume element of the Bures metric is, then,

$$\frac{\sqrt{15}\sqrt{1-21\zeta_{11110}^2}}{2\sqrt{-1+3\zeta_{11110}}\sqrt{1+3\zeta_{11110}}\sqrt{-1+5\zeta_{11110}}\sqrt{1+7\zeta_{11110}}}. \quad (38)$$

We have been unable, however, to either normalize this and/or derive a corresponding partition function.

III. QUANTUM CANONICAL ENSEMBLE FOR A CERTAIN THREE-LEVEL EXTENSION OF THE TWO-LEVEL SYSTEMS

In our final analysis, we apply the same line of reasoning utilized in the previous scenarios to recent results [21] concerning a particular *three*-level extension of the *two*-level systems. These were given by density matrices of the form,

$$\rho = \frac{1}{2} \begin{pmatrix} v+z & 0 & x-iy \\ 0 & 2-2v & 0 \\ x+iy & 0 & v-z \end{pmatrix}, \quad (39)$$

so for $v = 1$, the middle level is inaccessible and we recover the two-level systems. The normalized volume element of the associated Bures metric has been found to be [21, eq. (17)],

$$\frac{3}{4\pi^2 v \sqrt{1-v} \sqrt{v^2 - x^2 - y^2 - z^2}}. \quad (40)$$

From this, one can obtain (using spherical coordinates in the integrations), the univariate marginal distribution (an asymmetric beta distribution) over the interval $v \in [0, 1]$ [21, Fig. 3],

$$\frac{3v}{4\sqrt{1-v}}. \quad (41)$$

Interpreting this as the appropriate (normalized form of the) structure function, multiplying by the Boltzmann factor $e^{-\beta h v}$ and integrating the product over v from 0 to 1, we obtain the corresponding partition function,

$$Q(\beta) = \frac{3e^{-\beta h}((1+2\beta h)\sqrt{\pi}\text{erfi}(\sqrt{\beta h}) - 2\sqrt{\beta h}e^{\beta h})}{8(\beta h)^{3/2}}, \quad (42)$$

from which the thermodynamic behavior of an ensemble of such systems (39) can be deduced. For instance, the expected value of the “energy” ($h v$) is given by

$$-\frac{\partial \log Q(\beta)}{\partial \beta} = \frac{(4\beta^2 h^2 + 4\beta h + 3)\sqrt{\pi}\text{erfi}(\sqrt{\beta h}) - 2e^{\beta h}\sqrt{\beta h}(2\beta h + 3)}{2\beta((2\beta h + 1)\sqrt{\pi}\text{erfi}(\sqrt{\beta h}) - 2e^{\beta h}\sqrt{\beta h})}. \quad (43)$$

As $\beta \rightarrow 0$, this expected value approaches $\frac{4h}{5}$, while the variance about the expected value approaches $\frac{8h^2}{175}$.

IV. ANALYSES BASED ON THE MAXIMAL MONOTONE METRIC

Subsequent to the distribution of their original preprint [8], D. C. Brody kindly informed me that he and his co-author, L. Hughston, had “noticed that the phase space weighting used was incorrect, and as a result we find a different expression for the expected energy. Thus, although the claim of the paper is unchanged, we are now revising the example considered therein. Interestingly, the same (what we now believe is the correct) result was also predicted in our stochastic thermalisation model (quant-ph/9711057) — that is, instead of the ratio of the Bessel functions, $\frac{I_2}{I_1}$, we found the result given by the Langevin function.”

In a second message (also prior to the appearance of [7]), Brody wrote: “The only change [in [8]] we had to make is to replace the ‘phase space volume’ by ‘state density’ (i. e. weighted volume). As a consequence, this results in changing the calculation involving the spin- $\frac{1}{2}$ example. Nevertheless the behaviour of the Langevin function is somewhat similar to that of the ratio of the Bessel functions (e. g., energy, heat capacity).”

This reassessment of Brody and Hughston is paralleled by the replacement of the *minimal* monotone metric by the *maximal* monotone metric (of the left logarithmic derivative), since the use of the latter (coupled with a limiting argument), in fact, leads to the Langevin function, that is the ratio $\frac{I_{3/2}}{I_{1/2}}$, and not $\frac{I_2}{I_1}$. (For a comprehensive treatment of monotone metrics and the “geometries of quantum states”, see [15].) Such a view would, in addition, be apparently consistent with an earlier study of the author [25]. There, it was found that the maximal monotone metric yielded a more “noninformative” (that is, more “neutral” or less “biased”) prior, for Bayesian analysis, than did the minimal monotone metric (cf. [27]). (In the thermodynamic context, we form posterior distributions by multiplying prior distributions by Boltzmann factors, while in the Bayesian context, posteriors are formed by multiplying prior distributions by the likelihoods of a certain *finite* set of outcomes.)

Let us elaborate somewhat upon these points. The volume elements of both the minimal and maximal monotone metrics over the three-dimensional convex set (“Bloch sphere”) of spin- $\frac{1}{2}$ systems are proportional to expressions of the form,

$$\frac{1}{(1 - \xi_1^2 - \xi_2^2 - \xi_3^2)^u}, \quad (44)$$

where $u = \frac{1}{2}$ in the minimal case, and $\frac{3}{2}$ in the maximal one [15, eq. (3.17)]. In the minimal case, (44) can be directly normalized over the Bloch sphere ($\xi_1^2 + \xi_2^2 + \xi_3^2 \leq 1$), and we are able to obtain univariate marginal probability distributions of the type,

$$\frac{2\sqrt{1 - \xi_1^2}}{\pi}. \quad (45)$$

Employing this result in Poisson’s integral representation of the modified spherical Bessel functions (cylinder functions of half integral order) [14,29], we recover the associated partition function (1), as originally reported by Brody and Hughston [8], and independently, Slater [14]. For $u = \frac{3}{2}$, (44) is *not* normalizable (that is, improper) over the Bloch sphere. However, it can be normalized over a three-dimensional ball of radius $R < 1$. Then, integrating out one of the three Cartesian coordinates (say, ξ_3) over this ball of radius R , we obtain the bivariate probability distribution,

$$\frac{(R^2 - 1)\sqrt{R^2 - \xi_1^2 - \xi_2^2}}{2\pi\sqrt{1 - R^2}(-1 + \xi_1^2 + \xi_2^2)(R\sqrt{1 - R^2} + (R^2 - 1)\sin^{-1} R)}. \quad (46)$$

In the limit $R \rightarrow 1$, this converges to the bivariate probability distribution,

$$\frac{1}{2\pi\sqrt{1 - \xi_1^2 - \xi_2^2}}, \quad (47)$$

over the unit disk ($\xi_1^2 + \xi_2^2 \leq 1$). Its two univariate marginal probability distributions over ξ_1 and ξ_2 are simply uniform distributions ($\frac{1}{2}$) over the interval $[-1,1]$. They, then, give rise (again, applying Poisson’s integral representation) to the Langevin function — as in the revision by Brody and Hughston (cf. sec. IIB). It is also of interest to note that if we *ab initio* set one of the coordinates to zero in the volume element for the minimal metric (44), then the thermodynamic properties in such a *conditional* case are identical to those found in the maximal monotone analysis. So, we have two independent ways of arriving at the revised (and final) result of Brody and Hughston.

We have, in fact, conducted several analyses parallel to those reported above in the main body of the paper, but based on the maximal, rather than minimal monotone metric. (To obtain the specific forms of the metric, we solved

— for the two-particle scenarios — sets of thirty-two linear simultaneous equations [28, eq. (4.26)].) We take this opportunity to report these results.

For the analysis of sec. II A, we arrived at a maximal monotone metric simply proportional to the minimal monotone metric ((12)-(14)) and, hence, the same normalized density-of-states (16) and partition function (17).

For the analysis of sec. II B, we obtained a volume element of the maximal monotone metric equal to

$$\frac{\sqrt{2}\sqrt{\zeta_{11}^2 + 2\xi_1^{(a)2} - 1}}{\sqrt{1 - \zeta_{11}^2}(1 - 4\xi_1^{(a)2} - \zeta_{11}^2)}. \quad (48)$$

Its integral over the domain of feasible values diverges, however, and we have not been able to derive results analogous to (23) and (24).

For the analysis of sec. II C, we arrive at precisely the same results as before, that is, (26) and (27). Similarly, we obtain no differences with the analysis of sec. II D.

For the three-particle analysis of sec. II E, the normalized volume element of the maximal monotone metric is (cf. (31)),

$$\frac{\sqrt{3}}{\pi\sqrt{1 - 3\zeta_{111}^2}}, \quad (49)$$

so that

$$Q(\beta) = I_0\left(\frac{\beta h}{\sqrt{3}}\right). \quad (50)$$

(In the minimal monotone or Bures metric analysis, on the other hand, we were unable to find an explicit formula for the partition function.) For the four-particle analysis of sec. II E, the analogous results based on the maximal monotone metric are precisely the same ((32) - (34)). The maximal-monotone-metric analysis of the five-particle scenario yielded the same outcomes ((49)-(50)) as the maximal-monotone-metric analysis of the three-particle scenario.

For the three-particle scenario of sec. II F, an analysis based on the maximal monotone metric yielded the same results ((35)-(37)). As before, we have not been able to compute the volume element for the associated four-particle scenario.

For the analysis of sec. III, corresponding to a certain three-level extension of the two-level systems, we obtain a volume element (cf. (40)),

$$\frac{1}{\sqrt{1 - v(v^2 - x^2 - y^2 - z^2)}}, \quad (51)$$

not proportional to (40). However, using spherical coordinates and a limiting argument (that is, integrating over the radial coordinate r from 0 to $\frac{v}{R}$, normalizing this result, and then letting $R \rightarrow 1$), it can be shown to yield precisely the same univariate marginal probability distribution (41) as for the analysis based on the Bures metric, and hence lead to the same partition function (42).

It would be of interest to attempt to find a characterization of those cases in which the maximal and monotone metrics are the same (and so, of course, are their volume elements) or, more generally (as in the three-level extension example), of the cases in which the metrics may not be identical, but the associated thermodynamic properties are, nevertheless, the same.

Let us further note that for the *five*-dimensional convex set of *quaternionic* two-level quantum systems, the volume elements of the maximal and minimal monotone metrics are proportional to expressions of the form (cf. (44), [30, eqs. (7),(20)]),

$$\frac{1}{(1 - \xi_1^2 - \xi_2^2 - \xi_3^2 - \xi_4^2 - \xi_5^2)^u}, \quad (52)$$

where $u = \frac{1}{2}$ in the minimal case and $\frac{5}{2}$ in the maximal case. We then find — again applying Poisson's integral representation to the univariate marginal probability distributions obtained from (52) — that in the minimal case, the expected energy is proportional to the ratio $\frac{I_3}{I_2}$ and in the maximal case (applying a similar limiting argument, as used to obtain (47)) to the ratio $\frac{I_{5/2}}{I_{3/2}}$. So, these results are quite analogous to those for the three-dimensional convex set of *complex* two-level quantum systems.

Let us note that the results for the minimal and maximal monotone metrics coincide for precisely those scenarios in which we are concerned with a mutually *commuting* set of density matrices. Then, the scenario is essentially *classical*, rather than quantum, in nature. Hence, the monotone metric — the one associated with the Fisher information — is simply *unique*. We will also point out that in a related analysis [22], we found the maximal monotone metric to be considerably more amenable to our (MATHEMATICA) computations than was the minimal monotone metric.

V. CONCLUDING REMARKS

As with the instance of a *single* spin- $\frac{1}{2}$ particle studied in [8,14] — giving the previously reported results (1) and (2) — the possible applicability (to *small* systems, in particular [7]) of the several quantum canonical ensembles presented in this letter, awaits experimental examination. (We should note that it is usually considered that entangled particles will decohere *before* they are thermalized, that is, entanglement will be lost on time scales short compared to those of thermal relaxation processes associated with energy exchange with the bath [34].)

Although we have examined a number of possible scenarios here, there is clearly much opportunity for further systematic exploration along related lines. In fact, in [22], we were able to assign a prior probability distribution of the form $\frac{15(1-a)\sqrt{a}}{4\pi\sqrt{b}\sqrt{c}}$ to the two-dimensional simplex of diagonal entries — a, b, c — of the eight-dimensional convex set of spin-1 density matrices. (The evident symmetry between these three entries had been broken by a particular transformation, suggested by work of Bloore [40].) Then, we obtained a spin-1 counterpart — [22, Fig. 4] — to the Langevin function ($\frac{I_{3/2}}{I_{1/2}}$). These results pertained not to the *minimal* monotone metric (which proved to be more computationally problematical), but only to the *maximal* one — which is the subject of sec. IV — and is consistent with the reassessment by Brody and Hughston [7] of their original work [8], as the maximal monotone metric applied to a single spin- $\frac{1}{2}$ system, yields the Langevin function. As noted above, this also accords with certain arguments of Lavenda [10, pp. 20, 193, 198], who contends that the Langevin function has a sound probabilistic basis, while the Brillouin function does not. Also, as previously pointed out, the maximal monotone metric has been shown in two separate analyses [25,27] to be more *noninformative* in character than the minimal monotone metric. Other information-theoretic properties of these metrics have been studied in [32] (cf. [33]).

This study might be viewed as an attempt to respond to the concluding admonition of Petz and Sudár [15, p. 2672] that “more than one privileged metric shows up in quantum mechanics. The exact clarification of this point requires and is worth further studies”. In particular, we have been concerned with evaluating the various thermodynamic implications of these monotone metrics.

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APPENDIX. Information Gains from Differing Possible Outcomes of Joint Spin Measurements

We avail ourselves of the several prior probability distributions (normalized volume elements of Bures metrics) reported in sec. II, to obtain the information gains for various outcomes of joint measurements of the partially entangled spin- $\frac{1}{2}$ particles. (we might also pursue similar analyses using the results of sec. IV, based on the maximal monotone metric.) We pass, in this manner, from thermodynamic considerations to ones of a fundamentally Bayesian nature. We follow a methodology previously employed for *unentangled* spin- $\frac{1}{2}$ particles [35].

We associate with each specific outcome of a joint measurement of the partially entangled particles, a likelihood function, the product of which with the prior distribution can be normalized to yield — *via* Bayes' rule — a posterior probability distribution. We then compute the information gain (Kullback-Leibler statistic) of the posterior with respect to the prior. The products of the gains and their corresponding likelihoods averaged over all the possible outcomes with respect to the prior, then, give the *expected* information gain.

For the scenario of sec. II A, if we measure the spins of particles a and b along the axis of polarization, and find them to disagree (that is, one spin “up” and the other, “down”), we gain $\log 3 - \frac{2}{3} \approx .431946$ nats of information, while if they agree (both spins either up or down), we gain considerably less, that is, $\log 6 - \frac{5}{3} \approx .125093$. (The likelihood to be used in the Bayes' rule of obtaining a disagreement is $\frac{(1-\zeta_{11})}{2}$, while that for an agreement is $\frac{(1+\zeta_{11})}{2}$. The expected information gain is .329662.) If after one agreement, we obtain a disagreement, then the information gain due to the second measurement is greater than that from an initial disagreement, that is, $\log 5 - \frac{16}{15} \approx .542771$. If, instead, there is a second agreement, the additional information gain due to that outcome is only .0427712 nats. Further, if an initial disagreement is followed by another, the gain is $\log \frac{5}{3} - \frac{2}{3} \approx .110826$, while if the initial disagreement is succeeded by an agreement, the gain is $\log 10 - \frac{31}{15} \approx .235918$.

If we were to alter the scenario of sec. II A, setting $\xi_1^{(b)}$ equal to the negative of $\xi_1^{(a)}$ rather than to $\xi_1^{(a)}$ itself (so that the spins would be anticorrelated), we anticipate obtaining the same expected information gains, but for the reversed situations. For example, the gain due to an initial agreement would be .431946 nats, and not .125093, which would be that associated with an initial disagreement, . . .

Contrastingly, for the scenario of sec. II B, the information gain from an initial agreement is the same as that for an initial disagreement, that is $\log 2 - \frac{1}{2} \approx .193147$, so this is also the expected gain. If a second measurement yields an outcome different from the first, the information gain from this measurement is $\log 3 - \frac{5}{6} \approx .265279$, while if the outcome of the second measurement is the same as the first, the gain is $\log \frac{3}{2} - \frac{1}{3} \approx .0721318$ nats.

For the scenario of sec. II D, an initial agreement of spin measurements of particles a and b along an arbitrary axis yields an information gain of .306853 nats (saturating the Holevo-type bound [38,39]), while an initial disagreement gives .0646381 nats. (The expected information gain is .145376 nats.) A second agreement yields .0680544 nats, while a second disagreement gives .0470689 nats. An agreement after an initial disagreement results in a gain of .427868 nats, while a disagreement after an initial agreement provides .0516789 nats.

There, of course, still remains the possibility of using positive-operator-valued measures (POVM's) and/or standard measurements on *multiple* copies of (partially) entangled systems of spin- $\frac{1}{2}$ particles [35–37]. Along similar lines, in [35] it was found (based on the corresponding Bures metric) that for a pair of identically prepared *unentangled* spin- $\frac{1}{2}$ particles, one could expect to gain: (a) .357229 nats of information with the use of a particular POVM proposed by Peres [37] (having a continuum of possible outcomes); (b) .313478 nats for a certain joint measurement scheme of Popescu and Massar [36] (cf. [41,42]), having four possible outcomes; (c) .280372 nats if the spins of the two particles were to be measured separately in orthogonal directions; and (d) .212642 nats if measured separately in the same direction. A spin measurement on a *single* spin- $\frac{1}{2}$ particle can be expected to yield $.140186 = \frac{.280372}{2}$ nats [35].